

Dimethyl ethylmalonate
26717-67-9 | DTXSID70181214

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.54e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.16e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>ethyl 2-acetyloxypropanoate</div> <div>Measured: 2.00e-01</div> <div>Predicted: 2.26e-01</div>	<div>Image not found</div> <div>Propanoic acid, 2-(1-oxopropoxy)-, methyl ester</div> <div>Measured: 1.37e-01</div> <div>Predicted: 2.58e-01</div>	<div>Image not found</div> <div>2-Propene-1,1-diol diacetate</div> <div>Measured: 5.69e-02</div> <div>Predicted: 1.05e-01</div>
<div>Image not found</div> <div>Propylene glycol diacetate</div> <div>Measured: 6.24e-01</div> <div>Predicted: 3.94e-01</div>	<div>Image not found</div> <div>Diethyl maleate</div> <div>Measured: 8.13e-02</div> <div>Predicted: 9.69e-02</div>	